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DE-FG07-04ID14587

**AWARDEE NAME:**
University of Arizona

**PROJECT OR AWARDEE ACCOUNT NO:**
Acct. 340780

**PROJECT TITLE:**
Time-Dependent Neutral Particle Transport Benchmarks in Two and Three Dimensions

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**Report category:** Management
**Report name:** Final Report
**Period covered:** Aug 15, 2004 - June 14, 2007

## SUMMARY

The main objective of **NEER** grant **DE-FG07-04ID14587** was to generate highly accurate 2D and 3D time-dependent neutral particle intensity maps from 3D pulsed wire sources through integration of the analytical representation of a time-dependent point source. These maps would then serve as benchmark solutions for time-dependent transport methods developer. During the three years of this grant, we have shown that, in principle, any 3D wire source in an infinite medium can be simulated in this way. Year 1 was primarily concerned with the theory for 1D and 2D sources. The solution approach is rather novel in that the multidimensional solutions are based entirely on a 1D solution. In particular, a time-dependent point source is integrated over the wire source. For this reason, the point source solution had to be efficiently programmed to be as fast and accurate as possible, since it was to be at the center of a time consuming integration. The original point source solution was based on a multiple collision formulation which, by any measure, was entirely too slow for the intended use. Thus, the solution methodology was changed to a double

transform inversion, which gives the multiple collision series in summed form. One inversion could be performed analytically while the other required numerical quadrature. A new concept was then used in the numerical quadrature. In particular, since the inversion was essentially a Laplace transform inversion, the integrand, while real, was set in the complex plane. The evaluation proceeded by evaluating the integral through complex computer arithmetic giving its numerical value explicitly rather than first finding the integrand analytically. This proved to be an extremely efficient method of computation. With the help of then graduate student Roberto Furfaro, the 1D solution was tested against previous solutions developed some thirty years ago to ensure proper programming and extreme accuracy. At the end of Year 1 and during Year 2, numerical implementation of the integration over the wire source configuration was initiated. During this period, Roberto and I discovered that the uncollided flux, which is given entirely analytically, gave us difficulty because its extent had to be known exactly on the edit grid. This was because particles are emitted as a pulse and therefore there is a direct correlation between time and position. This requirement was also evident in determining what part of the source contributed to the intensity at a specific edit point. If the time elapsed since emission is insufficient for the entire source to have contributed, then the fraction that has contributed must be determined. This manifests itself as finding the appropriate limits of integration over the wire source. Effectively, a circle, with the edit point as its center, is drawn and the integration limits are where the circle cuts the source. The difficulty is to determine the correct direction of integration by just knowing the points of intersection. Unfortunately, the situation becomes more complicated when the edit point is out of the source plane. In any case, we were able to implement successfully several two- and three-dimensional sources, which impressively demonstrated the solution methodology. One of the difficulties is that finding these limits must be performed individually for each source. Year 2 ended with implementation of five one- and two-dimensional sources including the shell, solid sphere, finite line, circle and an ellipse. The implementation included testing in many ways possible, including interrogating perpendicular planes and confirming symmetries and intuition.

With the experience of one and two-dimensional sources, we were now ready to begin the implementation of 3D sources in an infinite medium. We began by considering a half circular pulsed source and then continued to pulsed broken wire sources, which were reported on in the Year 3 report. In addition, to these sources, we considered a helical wire source with eight windings.  Roberto, with the help of **MATLAB,** was able to animate some of these sources.  Unfortunately, they could not be included in this report because of the memory required and that this report must be e-mailed.

During the third year, the concept of iterative interpolation took shape and was applied in this and other projects.  This is a novel concept to reduce greatly the computational effort required by 3D source configurations.  In this concept, the point source is evaluated at only a few points for all edit points to be interrogated.  This was accomplished by first finding the maximum and minimum distances form all source points to all desired edit points.  Then, since the flux contribution from each point on the source depends on the relative difference between positions, and not on the absolute positions themselves, only a limited number of point sources are required for the integration.  This is accomplished by interpolating a set of base (usually 10) point sources to evaluate the integral over the wire source.  A fixed number of interpolations is set and then increased by two until the flux at all edit points has converged.  It was shown that high accuracy is maintained so the calculation can still be considered a benchmark.

A by-product of the work performed under this grant was the derivation of explicit analytical solutions for the 3D time-dependent transport equation.  While this is more a curiosity than a practicality, it does however add to the theoretical literature.  The solutions can be written in terms of integration of a point source giving an analytical representation in terms of several integrals.  It must be emphasized that it is the evaluation of these integrals that provides the practicality coming from this **NEER** grant.

Finally, there have been several consequential spin-offs from the work performed.  These include the following:

+ **Improved numerical Laplace transform**
The numerical Laplace transform can be a powerful numerical tool for solving linear equations with constant coefficients.  For example, the numerical inversion has been instrumental in solving the reactor kinetics equations including delayed neutrons.  We can apply the numerical Laplace transform inversion to the simplest of time-dependent transport scenarios.

+ **Convergence accelerated finite difference solution of the point kinetics equations**

Here, the concept of convergence acceleration is applied to a series of finite difference solutions to the point kinetics equations, which now form a sequence. The Wynn-epsilon (We) accelerator is used to accelerate the series sequence to convergence. Publication 10 details this analysis.

+ **Convergence acceleration and steady state with time-dependence**
Convergence acceleration was also applied to steady state numerical **SN** and **FN** algorithms as well as the one- and two- dimensional diffusion equation--with remarkable success. With such success, we have submitted a paper to the upcoming *Physor* '08 meeting attempting convergence acceleration in both time and space.

**Final Note**
The potential of much of what we have accomplished in this **NEER** project has yet to be fully realized. In particular, the application of parallel processing would make the research discoveries made many times more valuable.

## List of Publications

The publications listed are either directly related to or stimulated by the work performed under **NEER Grant DE-FG07-04ID14587**.


1. "Yet another Variation of the 1D Discrete Ordinates Algorithm of Neutron Transport", *Trans. Am. Nucl. Soc.* **91**, (2004).

2. "Progress Report on the Development of Time Dependent Neutral Particle Transport Benchmarks in Two and Three Dimensions", *Trans. Am. Nucl. Soc.* **93**, 458 (2005).

3. "Probabilistic and Generalized Regression Neural Networks for non-Multiplying Material Identification, (with R. Furfaro), *Trans. Am. Nucl. Soc.* **93**, 514 (2005).

4. "Can a Numerical Laplace Transform Inversion be Applied to the Reactor Kinetics Equations in Cylindrical Geometry?, A collection of papers dedicated to Silvio E. Corno, 115 (2005).

5. "A new 1D-Multigroup-Discrete Ordinates Algorithm for Neutron Transport", XIV ENFIR Conf, Santos, SP Brasil, Aug. 28-Sept 2, (2005).

6. “Mining the Multigroup Discrete Ordinates Algorithm for High Quality Solutions” (with D. E. Kornreich), Paper No. 7, ANS/M&C Topical Meeting, Avignon, France (2005).

7. “Multigroup 1D Homogeneous Medium Benchmark Using the Green’s Function Method” (with D. E. Kornreich), Paper No.61, ANS/M&C Topical Meeting, Avignon, France (2005).

8. “FN Approximation of the Solution to a Singular Integral Equation of Classical Reactor Physics”, *Ann. Nucl. Ener.*, Vol. **17**, 2017-2024 (2004).

9. “Thermal Neutron Diffusion in an Array of Plates”, B. Ganapol, *Nucl. Sci.& Eng*. **152**, 284-291 (2006).

10. “A further comment on “A Resolution of the Stiffness Problem of Reactor Kinetics” or “It’s all about nothing?”, B. Ganapol, Letter in *Nucl. Sci. & Eng*, 10/07.

11. “A Neutron Transport Benchmark in 1D Cylindrical Geometry: Revisited”, B.D. Ganapol, In Press *Nucl. Sci. and Eng*., 2007.

12. “Verification of the INL/**Combine7** Neutron Energy Spectrum Code, Barry D. Ganapol, Woo Y. Yoon, David W. Nigg, submitted to *Physor* ’08.

13. “Optimization of the Extrapolated Iterative Method for the Multislab Transport Problem”, Paolo Picca, Barry D. Ganapol and Roberto Furfaro, submitted to *Physor* ’08.

14. “Acceleration of the Numerical Solution of the Reactor Kinetics Equations in Plane Geometry”, B. D. Ganapol and E. H. Mund, submitted to *Physor* ’08.

15. “A 2D Benchmark for the Verification of the **PEBBED** Code”, Barry D. Ganapol, Hans A. Gougar and A.O.Ouguoag, submitted to *Physor* ’08.

16. “Inverse Point Kinetics with Neural Network”, Paolo Picca, Roberto Furfaro, Barry D. Ganapol, submitted to *Physor* ’08.

## The Time-Dependent 3D-Transport Source Gallery

**Fig. 1a The Spherical shell Source near rarefaction**

A spherical shell source is located at $r$ =1*mfp* in an infinite spherical medium. The pulse moves out into the expanse of the medium and simultaneously towards the center.

**Fig. 1b Rarefaction "wave"**

As the particles focus at the center, the flux distribution increases without bound sending a rarefaction wave outward. This is clearly seen.

**Fig. 1c Comparison of point and shell sources**

In this figure, we compare a point source at the center of the infinite medium with the above shell source at large time. As one expects, the two become coincident at large distance and times.

**Fig. 2 Comparison of point and spherical sources**

In this figure, we compare a point source and a spherical source of radius 1*mfp*. The intensities become nearly the same at large distance and times.

**Fig.3a Emission from a line source**

Here, we see the emission from a line source computed with the method of iterative interpolation. The pattern in the second plate is from the first collided contribution.

**Fig. 3b Relative error in iterative interpolation**

The relative error of the iterative interpolation is displayed here. The relative error is below $10^{-4}$ for less than 20 interpolants.

**Fig.4a Pulsed circular ring source**

A pulsed circular ring source is shown to emit into the infinite medium and toward the center

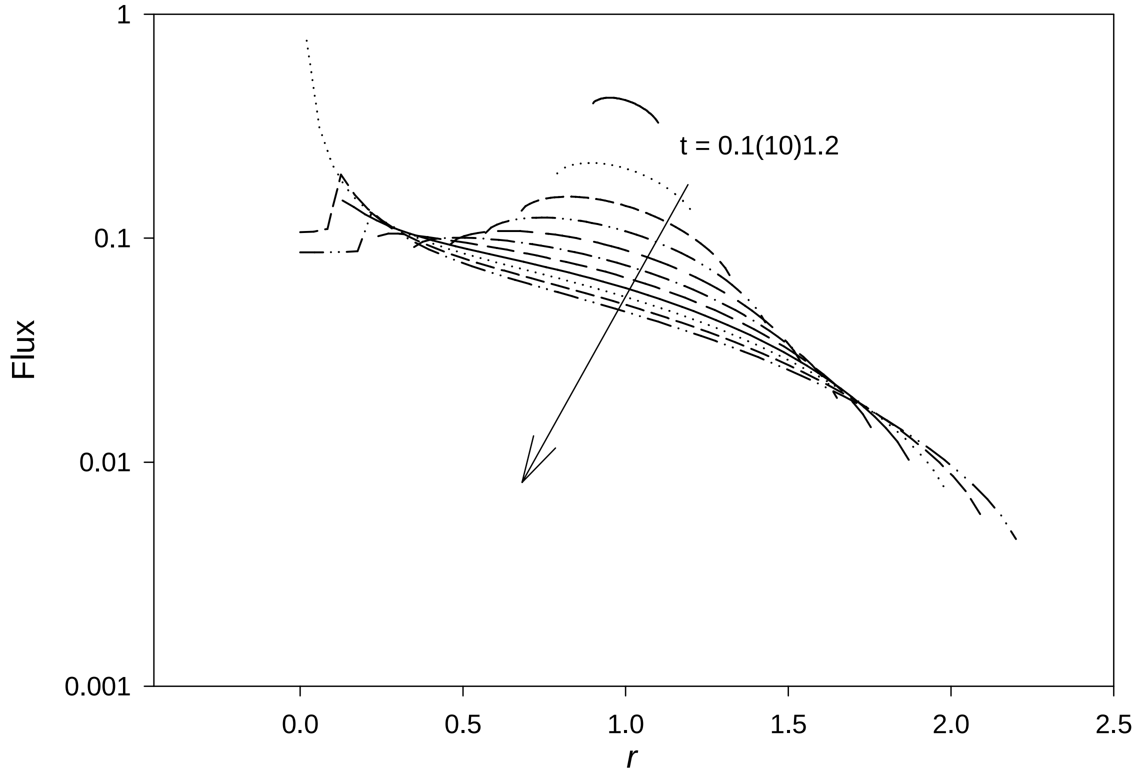
**Fig4b Pulse moving through center**

A close-up of the pulse moving through the center and back out is shown here. This figure indicates a particular advantage of an analytical solution as any region can be depicted without regard to the surrounding regions.

**Fig. 5 Semi-circular pulsed source**

The final figure in this gallery shows a semi-circular pulsed source. The 3D nature of this pulse is clear. Eventually, however scattering equilibrates the intensity and the 3D nature disappears.

Fig. 1a Spherical shell source ($a$ = 1) near rarefaction



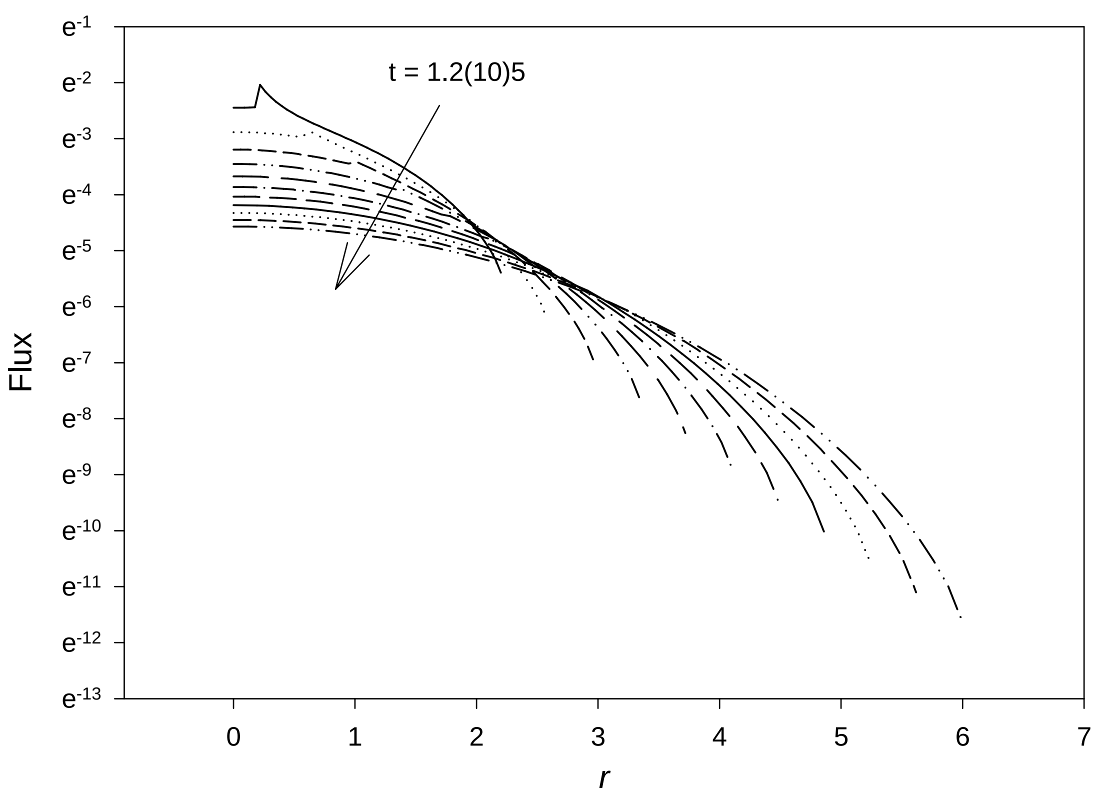



Fig 1b "Rarefaction" wave

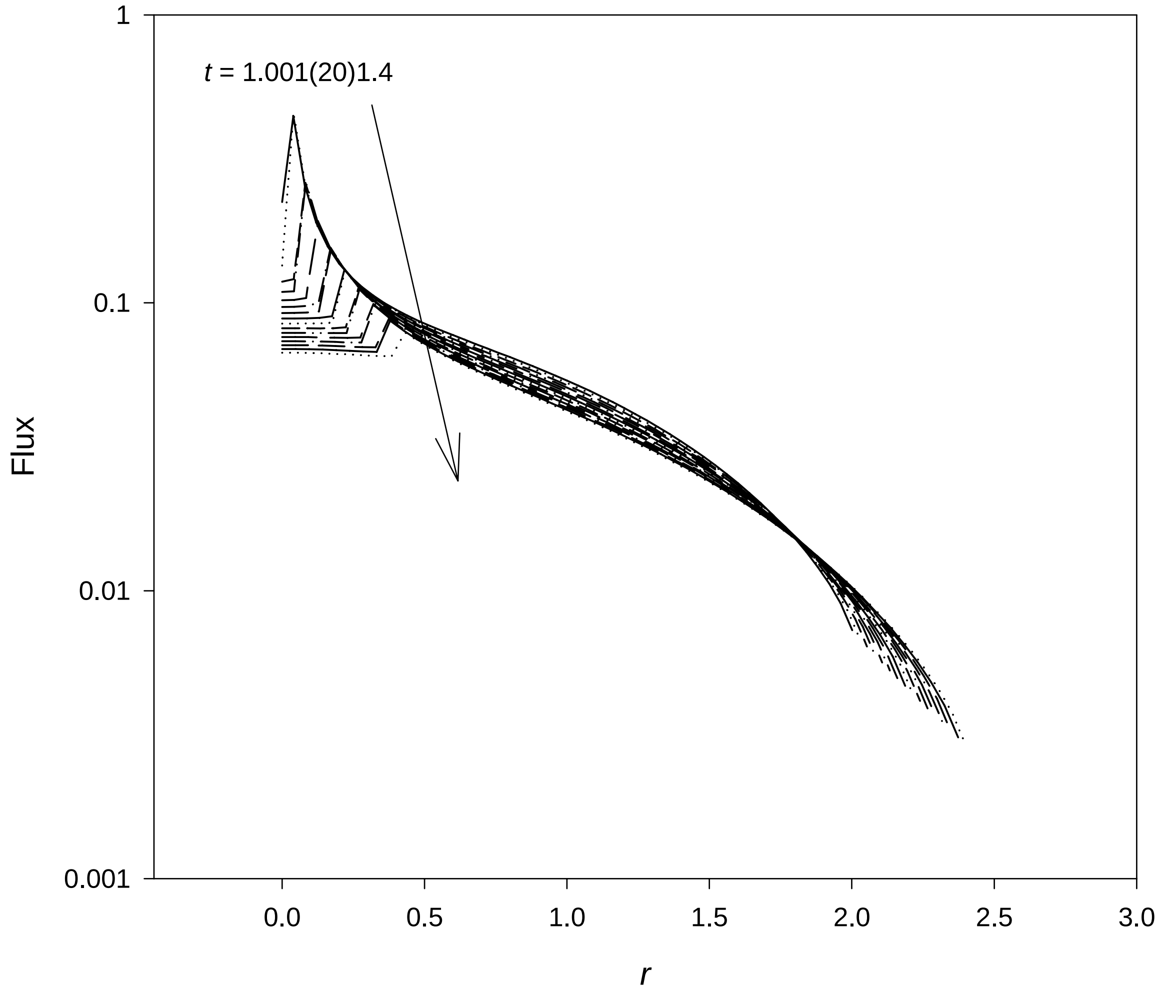
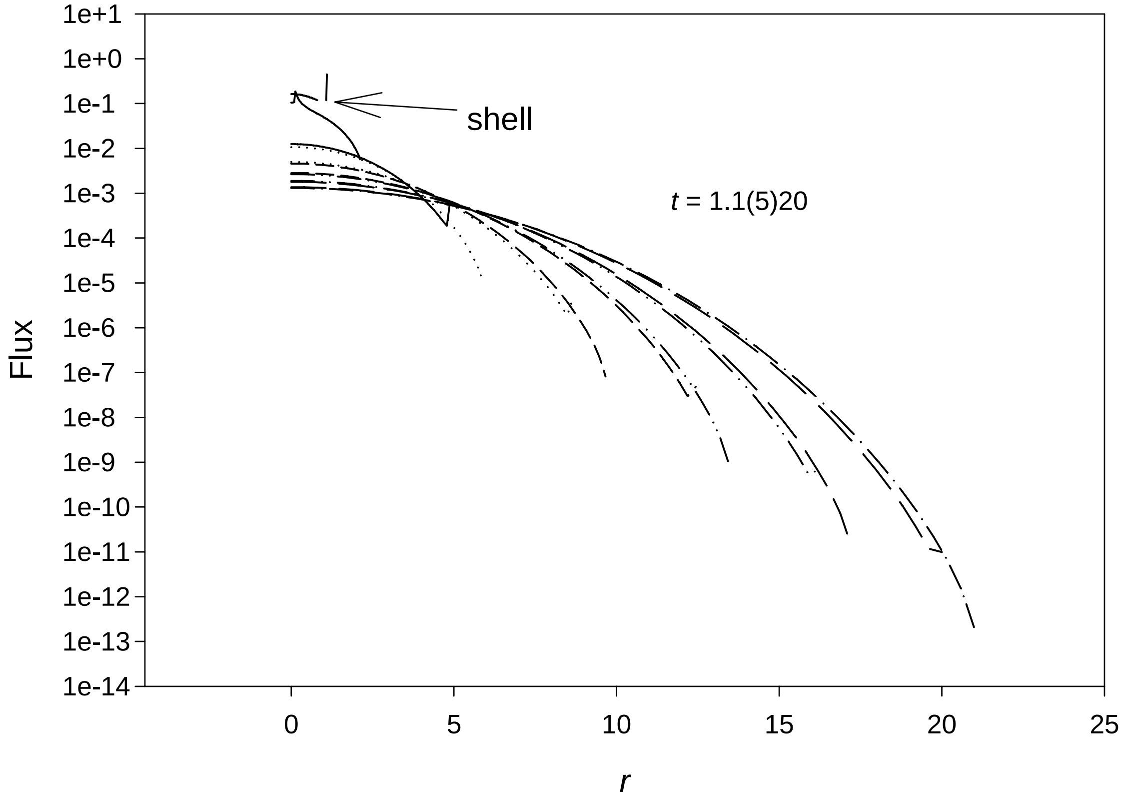


Fig 1c Comparison of point and shell sources



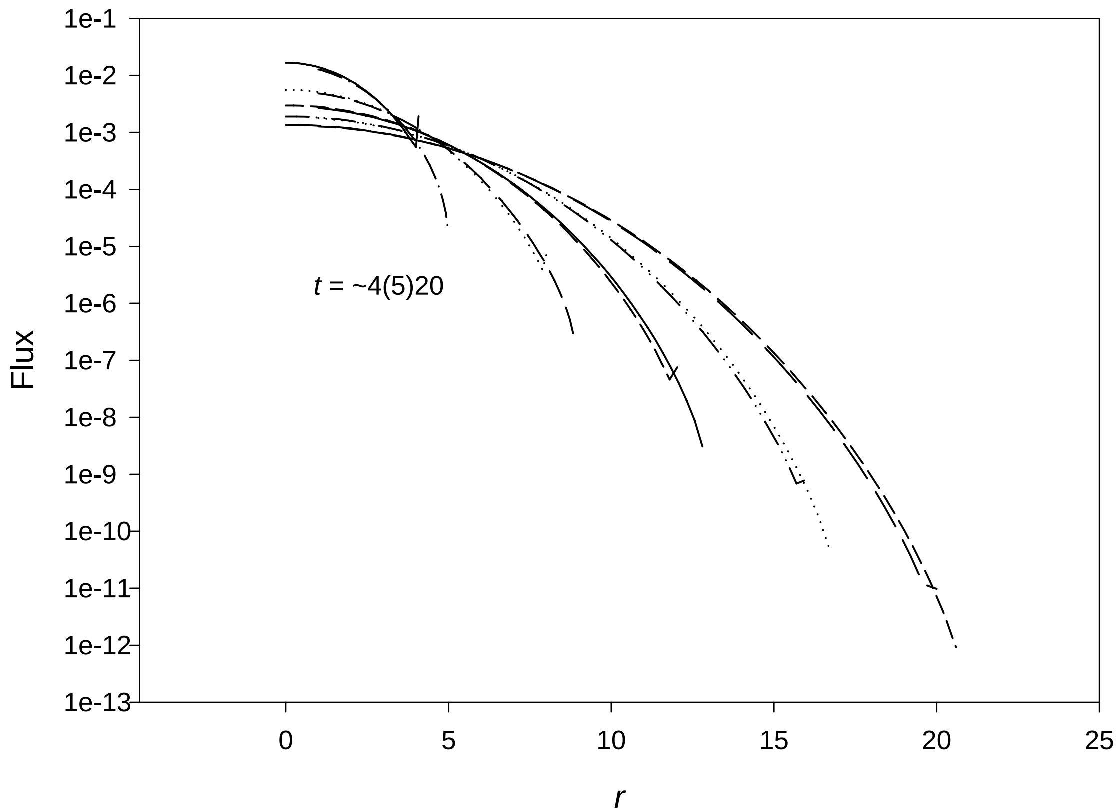



Fig. 2 Comparison of point and spherical sources (trace)

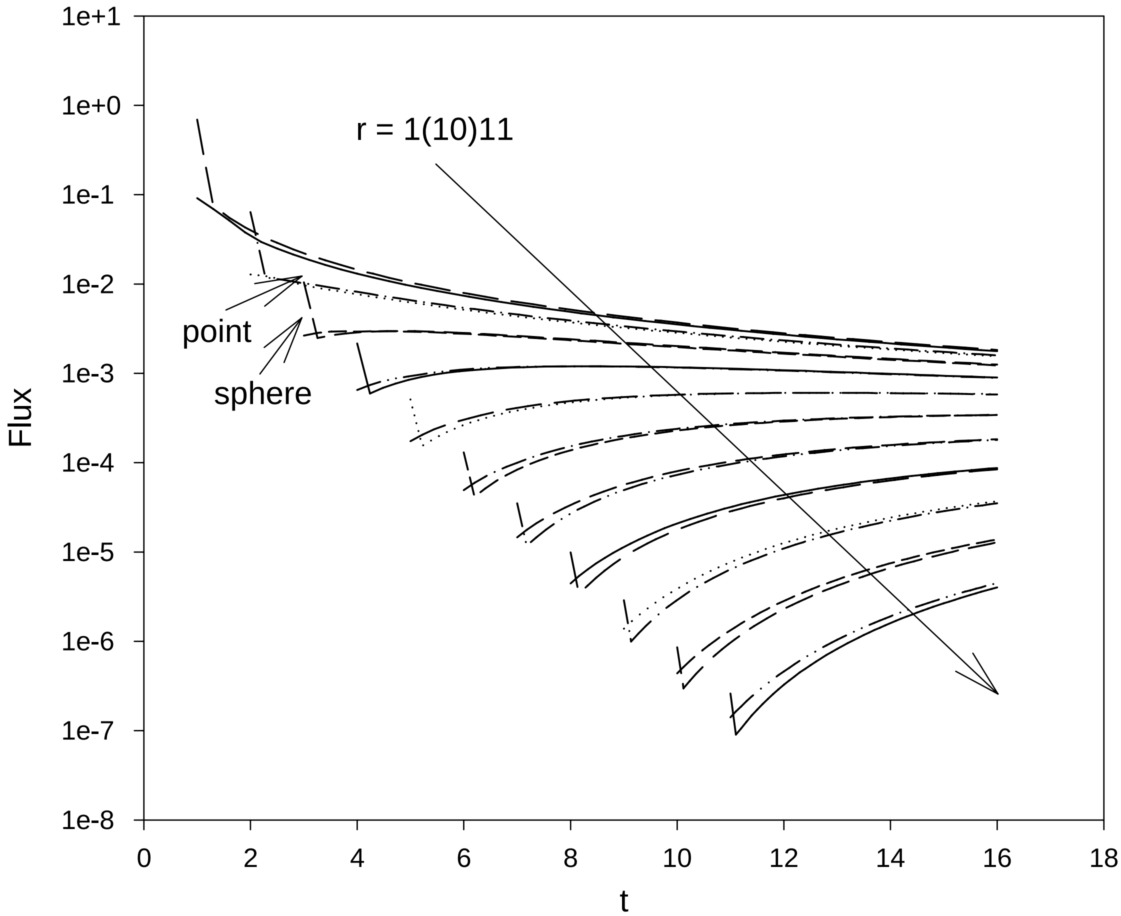


Fig. 3a Emission from a line source ($c$ = 1)

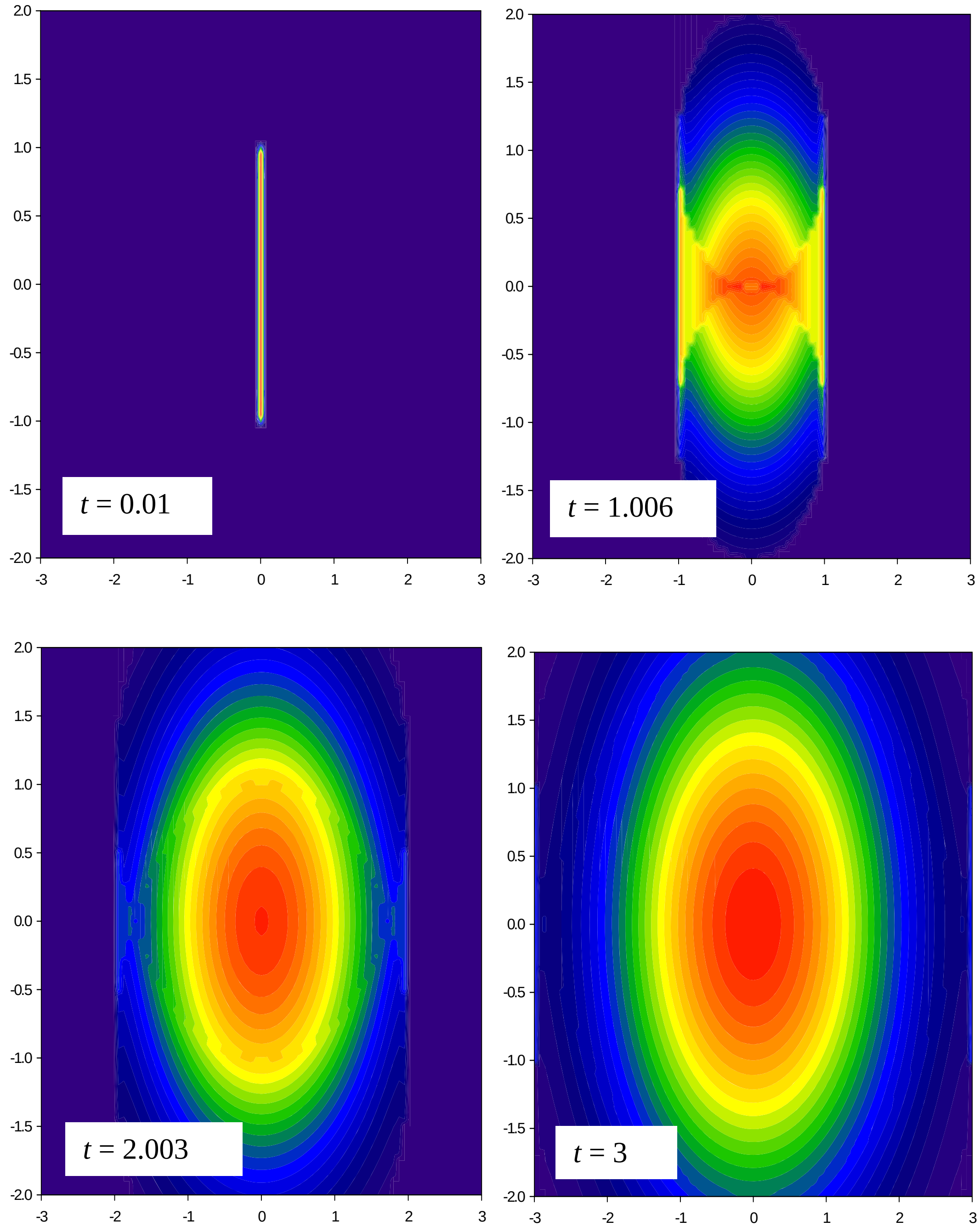
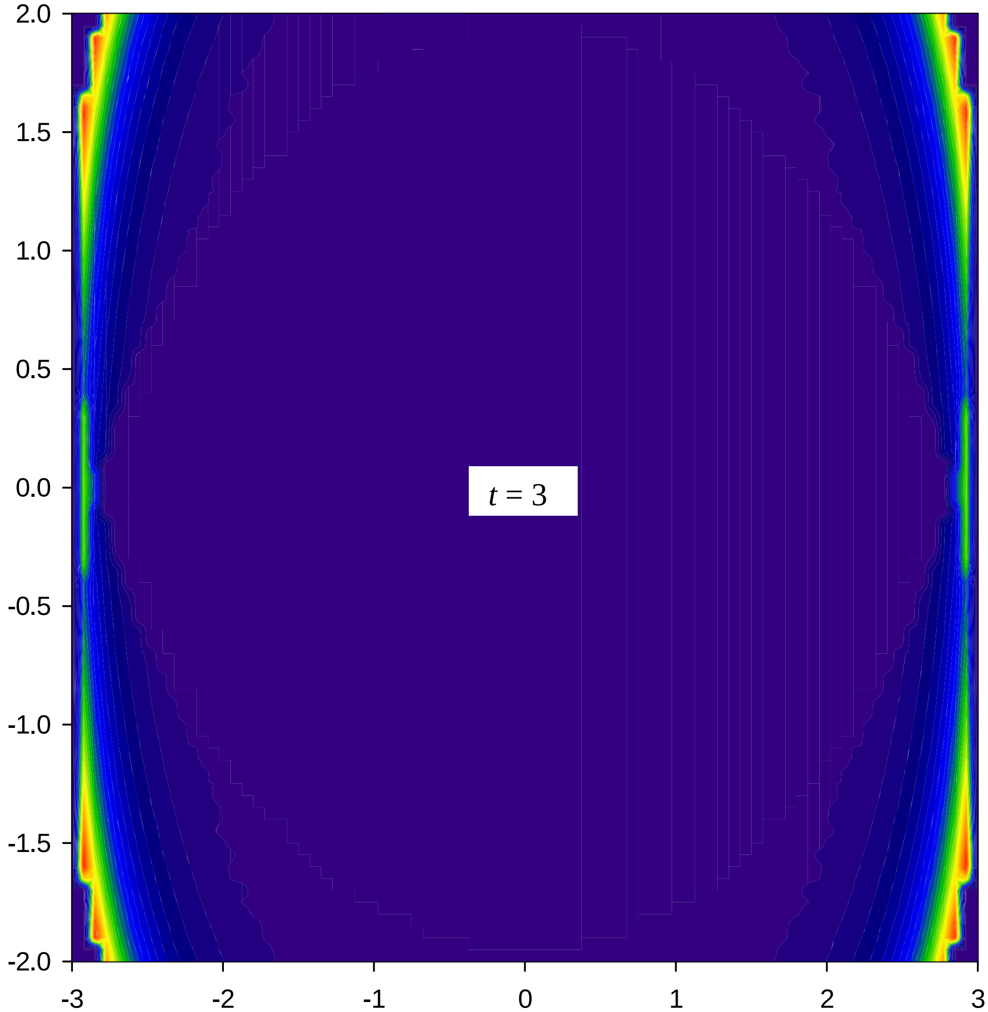


Fig. 3b Relative error in iterative interpolation



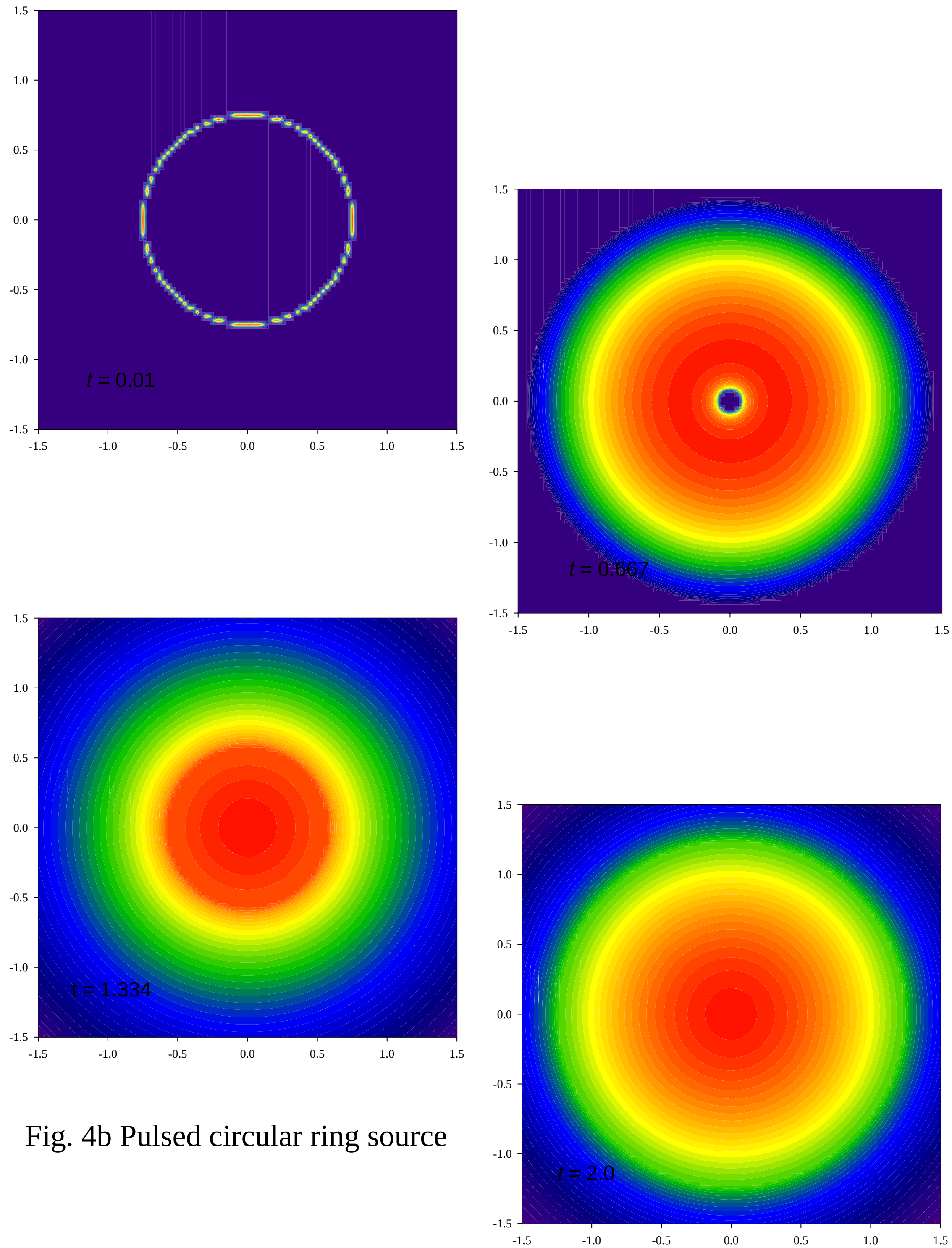



Fig. 4b Pulsed circular ring source

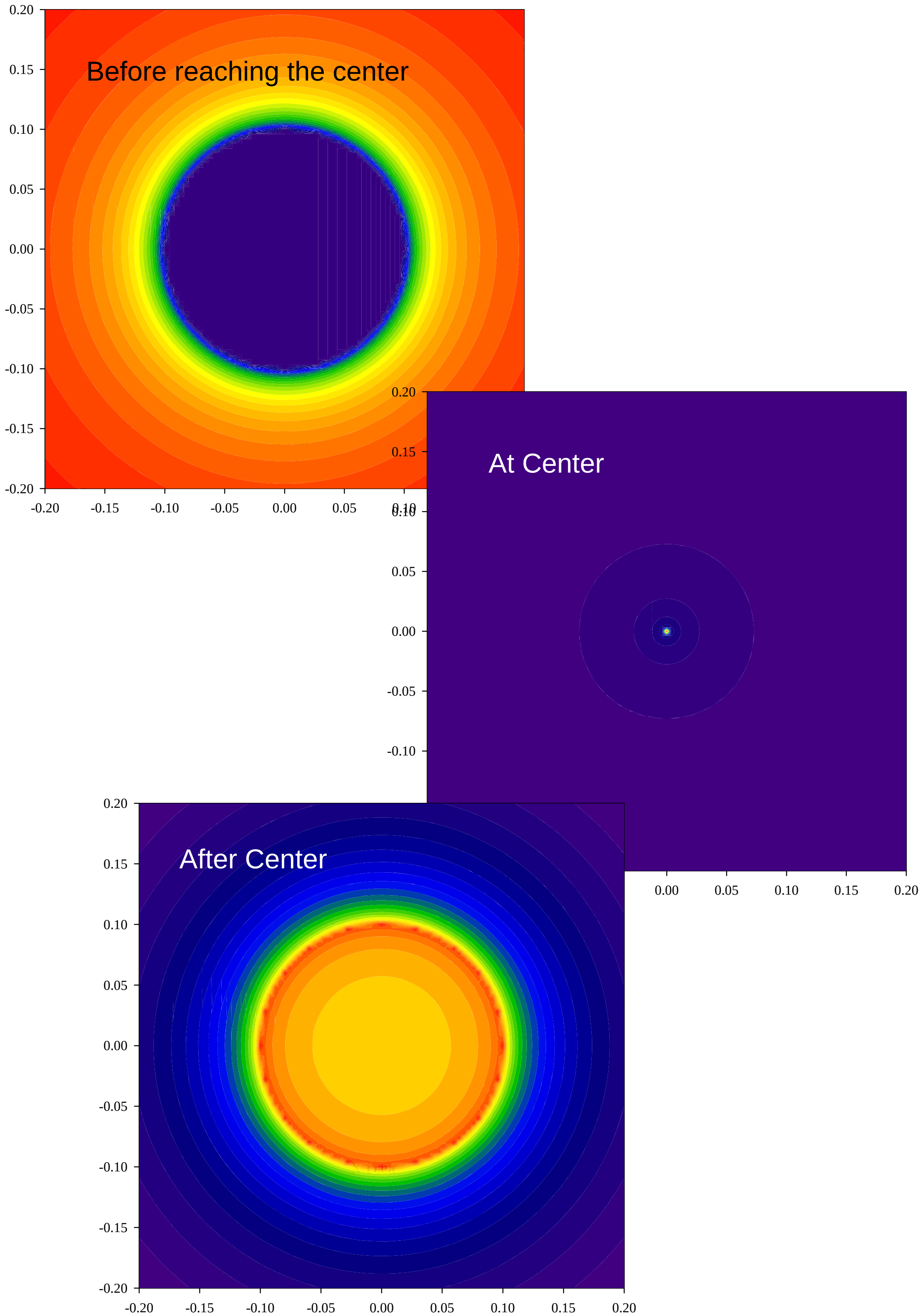



Fig. 4b Pulse moving through center

## Fig.5 Semi-circular pulsed source